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1. 1. cyclodextrin

Image: View the chemical structure

Definition:

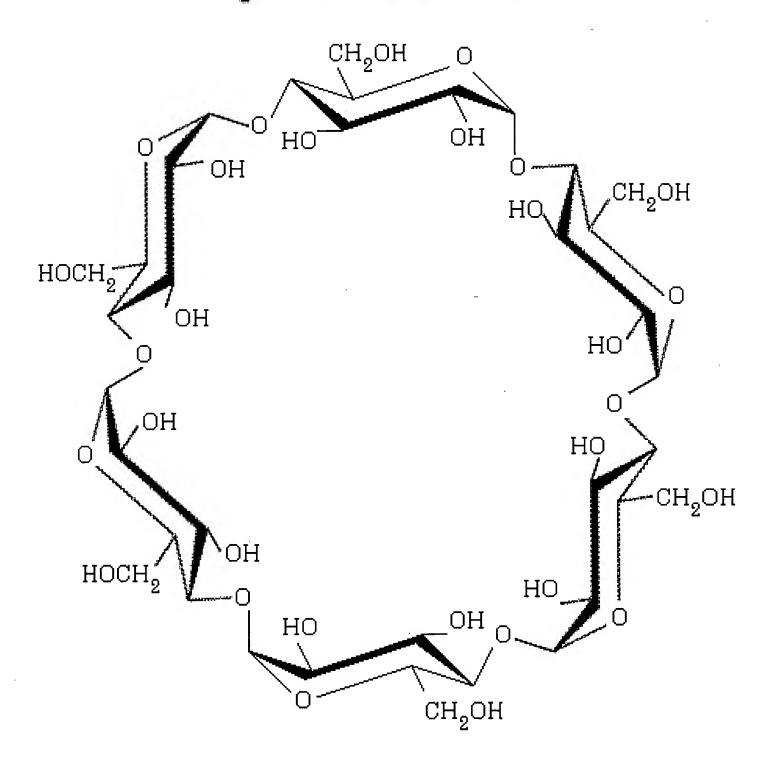
A cyclic <u>oligomer</u> of alpha-D-glucopyranose. The most common cyclodextrins are alpha, beta and gamma cyclodextrin having 6,7 and 8 glucopyranose units respectively. They occur naturally in starch digests of the bacteria *Bacillus Macerans*. With a <u>hydrophobic</u> interior cavity, they can complex small hydrophobic molecules while remaining soluble in water. Potential applications include water-soluble pharmaceuticals and herbicides and <u>pesticides</u>.

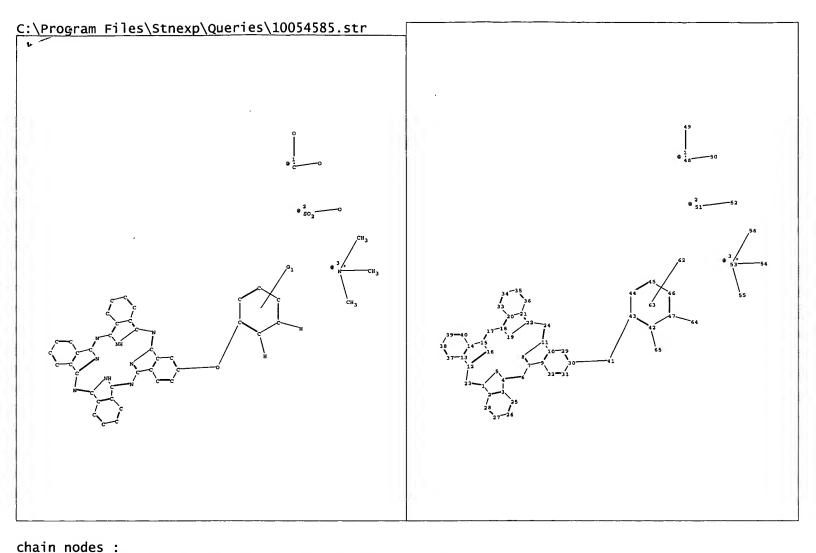
END

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1 of 1

cyclodextrins





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41 48 49
                    50 51 52
                                     53
                                         54
                                                55
                                                     56 62
ring nodes :
     1 2 3 4
                                     9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25
                        6
                                8
     26 27 28
                     29 30 31
                                                    35
                                     32
                                                         36 37 38 39 40 42 43 44 45 46 47
                                          33
                                               34
chain bonds :
                                         48-49 48-50 51-52 53-54 53-55
     30-41 41-43 42-65 47-64
                                                                                         53-56
ring bonds :
                                                                                         8-11 9-10 9-32 10-11
15-16 15-17 17-18 18-
27-28 29-30 30-31 31-
                                          3-4 3-25 4-5 4-6 6-7 7-8 7-9
12-23 13-14 13-37 14-15 14-40
21-22 21-36 22-24 25-26 26-27
              -5 1-23 2-3
11-24 12-13
19-22 20-21
                                 2-28 3-4 3-25 4-5
12-16 12-23 13-14
     1-2 1-5
                                                                                                                      18-19
              19-22
                        20-21
                                 20-33
     18-20
                                                                                                                      31-32
                                                                                         44-45 45-46 46-47
     33-34 34-35 35-36
                                 37-38 38-39 39-40
                                                            42-43
                                                                      42-47
                                                                              43-44
exact/norm bonds :
     1-5 4-5 18-19 19-22 30-41 41-43 48-49 48-50 51-52
exact bonds :
     42-65 47-64 53-54 53-55 53-56
normalized bonds :
                                 1-2 1-23 2-3
                          2-28
     12-13 12-16 12-23
21-22 21-36 22-24
                                         43-44 44-45
              39-40 42-43
                                                             45-46
                                                                      46-47
                                42-47
G1: [*1], [*2], [*3]
Match level:
     1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom 45:Atom 46:Atom 47:Atom 48:CLASS 49:CLASS 50:CLASS
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51:CLASS 52:CLASS 53:CLASS 54:CLASS 55:CLASS 56:CLASS 62:CLASS 63:CLASS 64:CLASS

65:CLASS

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=> file reg

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION

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TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

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Uploading 10054585.str

L1 STRUCTURE UPLOADED

=> s l1

SAMPLE SEARCH INITIATED 14:54:50 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 6 TO ITERATE

100.0% PROCESSED 6 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 6 TO 266

PROJECTED ANSWERS: 0 TO 0

=> s l1 sss full

FULL SEARCH INITIATED 14:55:07 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 314 TO ITERATE

5 ANSWERS

100.0% PROCESSED 314 ITERATIONS

SEARCH TIME: 00.00.01

L3 5 SEA SSS FUL L1

=> d ide cbib pi 1-5

L3 ANSWER 1 OF 5 REGISTRY COPYRIGHT 2002 ACS

RN 177992-33-5 REGISTRY

CN Benzoic acid, 4,4',4'',4'''-[29H,31H-phthalocyanine-2,9,16,23-tetrayltetrakis(oxy)]tetrakis-, tetrakis(2-ethylhexyl) ester (9CI) (CA INDEX NAME)

MF C92 H98 N8 O12

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

PAGE 1-A

PAGE 1-B

$$\begin{array}{c|c} \text{O} & \text{Et} \\ \parallel & \parallel \\ \nearrow \text{C--O-CH}_2\text{--CH-Bu-n} \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1962 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 125:37859 Method for tagging petroleum products. Krutak, James John; Cushman, Michael Roy; Weaver, Max Allen (Eastman Chemical Company, USA). PCT Int. Appl. WO 9610620 A1 19960411, 87 pp. DESIGNATED STATES: W: BR, CA, CN, HU, JP, KR, MX, NO, PL, RU; RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1995-US12191 19950925. PRIORITY: US 1994-315386 19940930. PATENT NO. KIND DATE APPLICATION NO. DATE

PI WO 9610620 A1 19960411 WO 1995-US12191 19950925
W: BR, CA, CN, HU, JP, KR, MX, NO, PL, RU
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE
US 5525516 A 19960611 US 1994-315386 19940930
US 5525516 B1 19991109

ZA 9508247 A 19960424 ZA 1995-8247 19950929

L3 ANSWER 2 OF 5 REGISTRY COPYRIGHT 2002 ACS

RN 177992-10-8 REGISTRY

CN Benzoic acid, 4,4',4'',4'''-[29H,31H-phthalocyanine-2,9,16,23-tetrayltetrakis(oxy)]tetrakis-, tetrakis(2,2-dimethylpropyl) ester (9CI) (CA INDEX NAME)

MF C80 H74 N8 O12 .

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

PAGE 1-A

$$\begin{array}{c} \begin{array}{c} \begin{array}{c} \\ \\ \\ \\ \\ \\ \end{array} \end{array}$$

PAGE 1-B

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1962 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 125:37859 Method for tagging petroleum products. Krutak, James John; Cushman, Michael Roy; Weaver, Max Allen (Eastman Chemical Company, USA). PCT Int. Appl. WO 9610620 A1 19960411, 87 pp. DESIGNATED STATES: W: BR, CA, CN, HU, JP, KR, MX, NO, PL, RU; RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1995-US12191 19950925. PRIORITY: US 1994-315386 19940930. KIND DATE APPLICATION NO. DATE PATENT NO. _____ ____ _____ -----WO 1995-US12191 19950925 PIWO 9610620 **A1** 19960411 W: BR, CA, CN, HU, JP, KR, MX, NO, PL, RU RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE

US 5525516 A 19960611 US 1994-315386 19940930 US 5525516 B1 19991109 ZA 9508247 A 19960424 ZA 1995-8247 19950929 L3 ANSWER 3 OF 5 REGISTRY COPYRIGHT 2002 ACS

RN 177991-95-6 REGISTRY

CN Benzoic acid, 4,4',4'',4'''-[29H,31H-phthalocyanine-2,9,16,23-tetrayltetrakis(oxy)]tetrakis-, tetrakis(decyl) ester (9CI) (CA INDEX NAME)

MF C100 H114 N8 O12

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

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PAGE 1-B

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1962 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 125:37859 Method for tagging petroleum products. Krutak, James John; Cushman, Michael Roy; Weaver, Max Allen (Eastman Chemical Company, USA). PCT Int. Appl. WO 9610620 A1 19960411, 87 pp. DESIGNATED STATES: W: BR, CA, CN, HU, JP, KR, MX, NO, PL, RU; RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1995-US12191 19950925. PRIORITY: US 1994-315386 19940930.

PATENT NO. KIND DATE APPLICATION NO. DATE

PI WO 9610620 A1 19960411 WO 1995-US12191 19950925 W: BR, CA, CN, HU, JP, KR, MX, NO, PL, RU

RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE

US 5525516 A 19960611 US 1994-315386 19940930

US 5525516 B1 19991109

ZA 9508247 A 19960424 ZA 1995-8247 19950929

L3 ANSWER 4 OF 5 REGISTRY COPYRIGHT 2002 ACS

RN 174320-94-6 REGISTRY

CN Benzenaminium, 4,4',4'',4'''-[29H,31H-phthalocyanine-2,9,16,23-tetrayltetrakis(oxy)]tetrakis[N,N,N-trimethyl- (9CI) (CA INDEX NAME)

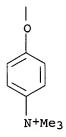
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SR CA

LC STN Files: CA, CAPLUS

PAGE 1-A

PAGE 2-A



1 REFERENCES IN FILE CA (1962 TO DATE)

1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 124:189103 Studies of the supramolecular system of porphyrin-phthalocyanine formed by molecular self-assembly and its photoinduced electron transfer processes. Tian, Hongjian; Zhou, Qingfu; Shen, Shuyin; Xu, Huijun (Institute Photographic Chem., Chinese Academy Sciences, Beijing, 100101, Peop. Rep. China). Wuli Huaxue Xuebao, 12(1), 44-8 (Chinese) 1996. CODEN: WHXUEU. ISSN: 1000-6818. Publisher: Beijing Daxue Chubanshe.

L3 ANSWER 5 OF 5 REGISTRY COPYRIGHT 2002 ACS

RN 147699-74-9 REGISTRY

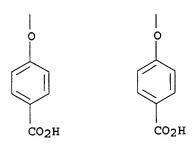
MF C88 H50 N8 O24

SR CA

LC STN Files: CA, CAPLUS, CASREACT

PAGE 1-A

PAGE 2-A



1 REFERENCES IN FILE CA (1962 TO DATE)

1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 118:254603 A simple synthesis of 4,5-disubstituted 1,2-dicyanobenzenes and 2,3,9,10,16,17,23,24-octasubstituted phthalocyanines. Woehrle, Dieter; Eskes, Marco; Shigehara, Kiyotaka; Yamada, Akira (Inst. Org. Makromol. Chem., Univ. Bremen, Bremen, D-2800/33, Germany). Synthesis (2), 194-6 (English) 1993. CODEN: SYNTBF. ISSN: 0039-7881.

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FULL ESTIMATED COST

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